

An analysis of the trigonal center structure of Yb³⁺ ion in CsCaF₃

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Abstract

© Springer-Verlag Wien 2014. The crystal field parameters determined from interpretation of optical spectra are used to analyze distortions of a crystal lattice in the vicinity of an impurity ion and vacancy at a Cs⁺ site compensating the excess positive charge in the trigonal centers of Yb³⁺ ions in CsCaF₃ crystal. Interactions of the impurity ion with the nearest neighbors (an octahedron of F⁻ ions) and the next nearest neighbors (a cube of Cs⁺ ions) are considered within the superposition model. It is established that, at formation of the trigonal center, three F⁻ ions of the nearest octahedron, placed symmetrically along the threefold axis on the side of the vacancy, move away from the impurity ion a little and significantly deviate from this axis. The second triangle of F⁻ ions, on the contrary, comes nearer to the impurity ion and nestles on the axis of the center a little. The three Cs⁺ ions, the second neighbors on the side of the vacancy, slightly come nearer to Yb³⁺ ion and considerably nestle on the center axis. The second triangle of Cs⁺ ions, from the opposite side of vacancy, also comes nearer to the paramagnetic ion and also nestles on the center axis a little. The Cs⁺ ion, lying on the center axis, comes considerably nearer to the impurity ion.

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